# The Lee-Huang-Yang formula for the ground state energy of Bose gases

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**Based on joint work with Jan Philip Solovej**

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# The dilute Bose gas

Consider $N$ interacting, non-relativistic bosons in a box $\Lambda := [-L/2, L/2]^3$. Let $N \in \mathbb{N}$, $\rho := N/|\Lambda| = N/L^3$.
The Hamiltonian of the system is, on the symmetric (bosonic) space $\otimes_s^N L^2(\Lambda)$,

$$H_N := \sum_{i=1}^{N} -\Delta_i + \sum_{i<j} v(x_i - x_j),$$

and $0 \leq v \in L^1(\mathbb{R}^3)$ is radially symmetric with compact support.

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The energy density in the thermodynamic limit is

$$e(\rho) = \lim_{L \to \infty, N/|\Lambda| = \rho} E_0(N, \Lambda)/L^3.$$

# The scattering length

**Scattering equation**

$$(-\Delta + \frac{1}{2}v(x))(1-\omega(x)) = 0, \qquad \text{with } \omega \to 0, \text{ as } |x| \to \infty.$$

**Scattering length**

$$a := \lim_{|x|\to\infty} |x|\omega(x) = \frac{1}{8\pi}\int v(1-\omega) < \frac{1}{8\pi}\int v =: a_1.$$

With $g = v(1-\omega)$ the scattering equation can be reformulated as

$$-\Delta\omega = \frac{1}{2}g, \qquad \text{i.e.} \qquad \widehat{\omega}(k) = \frac{\widehat{g}(k)}{2k^2}.$$

# The two-term formula

We study $e(\rho)$ in the dilute limit $\rho a^3 \to 0$. The following formula is expected to be true

$$e(\rho) = 4\pi\rho^2 a(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}) + \rho^2 a\, o((\rho a^3)^{1/2}).$$

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- Lenz (1929), Bogoliubov (1947), Lee-Huang-Yang (1957).
- Rigorous proof of leading term Dyson (1957, upper), Lieb-Yngvason (1998).
- Upper bounds giving second order term: Erdős-Schlein-Yau (2008), Yau-Yin (2009).
- Study of the limit for $v$ becoming 'soft' as $\rho \to 0$: Lieb-Solovej, Giuliani-Seiringer (2008), Brietzke-Solovej (2018).
- Bogoliubov theory for confined Bose gases (Gross-Pitaevskii limit) Boccato-Brennecke-Cenatiempo-Schlein (2017-2018).

# The Lee-Huang-Yang formula

**Theorem (SF, Solovej 2019)**

*Given a potential $v \neq 0$, non-negative, radial, $L^1$, with compact support there exist $C, \eta > 0$ (depending on $v$) such that for all $\rho$ sufficiently small,*

$$e(\rho) \geq 4\pi\rho^2 a\Big(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}\Big) - C\rho^2 a(\rho a^3)^{\frac{1}{2}+\eta}.$$

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Combined with the upper bound from Yau-Yin this proves the Lee-Huang-Yang formula for the ground state energy.

# Strategy of proof

- Localize to boxes of size $\ell \gg (\rho a)^{-\frac{1}{2}}$. Localization non-standard since need to preserve 'Neumann gap'. To get a priori information localize to smaller boxes of size $\lesssim (\rho a)^{-\frac{1}{2}}$. Here Neumann gap can be used to control errors. Rest of analysis carried out on large box. The interaction between localized particles is denoted by $w(x_i, x_j)$.
- Condensation. Let $P$ projection on constant function, $Q$ orthogonal complement.

$$n_0 = \sum P_i, \qquad n_+ = \sum Q_i.$$

A priori bounds control expected values $\langle n_0 \rangle$ and $\langle n_+ \rangle$. Energy error negligible if localizing to subspace where $n_+ \leq \mathcal{M}$, where $\mathcal{M}$ is of the order of the bound on $\langle n_+ \rangle$.

Clearly $1 = P_1 P_2 + Q_1 P_2 + P_1 Q_2 + Q_1 Q_2$.

# 2-particle terms/The 4Q term

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$$\begin{aligned} w(x_i, x_j) &= P_i P_j w P_j P_i + (Q_i P_j w P_j P_i + P_i Q_j w P_j P_i + h.c.) + \ldots + Q_i Q_j w Q_j Q_i \\ &= \{Q_i Q_j + (P_i P_j + P_i Q_j + Q_i P_j)\omega\}\, w\, \{Q_j Q_i + \omega(P_i P_j + P_i Q_j + Q_i P_j)\} + \ldots \end{aligned}$$

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So (all sums over $i \neq j$): $\frac{1}{2}\sum w(x_i, x_j) \geq \mathcal{Q}_0 + \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3'$,

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So (all sums over $i \neq j$): $\frac{1}{2}\sum w(x_i, x_j) \geq \mathcal{Q}_0 + \mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3'$, where

$$\begin{aligned} \mathcal{Q}_3' &:= \sum P_i Q_j w_1(x_i, x_j) Q_j Q_i + h.c. \\ \mathcal{Q}_2 &:= \sum P_i Q_j w_2(x_i, x_j) P_j Q_i + \sum P_i Q_j w_2(x_i, x_j) Q_j P_i \\ &\quad + \frac{1}{2}\sum (P_i P_j w_1(x_i, x_j) Q_j Q_i + h.c.), \\ \mathcal{Q}_1 &:= \sum P_j Q_i w_2(x_i, x_j) P_i P_j, \qquad \mathcal{Q}_0 := \frac{1}{2}\sum P_i P_j w_2(x_i, x_j) P_j P_i \end{aligned}$$

and where $w_1 = w(1 - \omega) \approx g$, $w_2 = w(1 - \omega^2) = w_1(1 + \omega)$.

# Strategy of proof II

- Discarding the positve $4Q$ term has renormalized the interaction. No "bare" $w$ appears.
- Rest of proof in 2nd quantization. For simplicity of presentation, we will assume periodic boundary conditions and $w = v$. Then $1Q$ terms disappear. In the real proof, $1Q$ terms are present and the cancelation of the $1Q$ terms has to be done carefully.

# Strategy of proof II

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  Standard bosonic creation/annihilation operators $a_k, a_k^\dagger$, $k \in (2\pi\ell^{-1})\mathbb{Z}^3$.
  $$[a_k, a_{k'}] = 0, \qquad [a_k, a_{k'}^\dagger] = \delta_{k,k'}.$$
- $c$-number substitution. Replace all $a_0, a_0^\dagger$ by $\sqrt{n}$.
  Expect $n_0 \approx n \approx \rho\ell^3 = K^3(\rho a^3)^{-\frac{1}{2}}$. So $1/n_0 \ll (\rho a^3)^{\frac{1}{2}}$.
- Localize $3Q$-term: A preliminary analysis allows cut-offs in the $3Q$-term to soft-pair interactions only.

# Diagonalizing the operator

Let $\mathcal{K}$ be the Hamiltonian on a periodic box, after $c$-number substitution

$$\mathcal{K} = \frac{1}{2}\rho^2\ell^3\widehat{g}(0) + \frac{1}{2}\rho^2\ell^3\widehat{g\omega}(0) + \mathcal{K}^{\rm Bog} + \mathcal{Q}_2^{\rm ex} + \mathcal{Q}_3.$$

Here, with $\mathcal{A}(k) := k^2 + \rho\widehat{w_1}(k)$, $\quad \mathcal{B}(k) := \rho\widehat{w_1}(k)$.

$$\mathcal{K}^{\rm Bog} := \frac{1}{2}\sum_k \Big(\mathcal{A}(k)(a_k^\dagger a_k + a_{-k}^\dagger a_{-k}) + \mathcal{B}(k)(a_k^\dagger a_{-k}^\dagger + a_k a_{-k}),$$

and (with $P_L$ being low momenta $\leq \sqrt{\rho a}$, $P_H$ high momenta $\approx a^{-1}$)

$$\mathcal{Q}_2^{\rm ex} := \rho\sum_k \big(\widehat{w_1\omega}(0) + \widehat{w_1\omega}(k)\big) a_k^\dagger a_k \approx 2\rho\widehat{w_1\omega}(0) n_+$$

$$\mathcal{Q}_3 := \ell^{-3}\sqrt{n} \sum_{k\in P_H, s\in P_L} \widehat{w}_1(k)(a_s^\dagger a_{s-k} a_k + a_k^\dagger a_{s-k}^\dagger a_s).$$

# Diagonalizing $\mathcal{K}^{\mathrm{Bog}}$ (The idealized Bogoliubov calculation)

$$(a_k^\dagger + \alpha_k a_{-k})(a_k + \alpha_k a_{-k}^\dagger) = a_k^\dagger a_k + \alpha_k^2 a_{-k}^\dagger a_{-k} + \alpha_k(a_k a_{-k} + a_k^\dagger a_{-k}^\dagger) - \alpha_k^2 [a_{-k}, a_{-k}^\dagger].$$

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$$= \sum_k \Big(\mathcal{D}_k b_k^\dagger b_k - (\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2})\Big)$$

where $b_k := a_k + \alpha_k a_{-k}^\dagger$, $\mathcal{D}_k = \frac{1}{2}(\mathcal{A}_k + \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx k^2$, and

$\alpha_k = \mathcal{B}_k^{-1}(\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2}) \approx \frac{\mathcal{B}_k}{2\mathcal{A}_k} \approx \rho\frac{\widehat{g}(k)}{2k^2} = \rho\widehat{\omega}(k)$ ($\approx$ valid for $|k|$ near $a^{-1}$).

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The constant term $\sum(\mathcal{A}_k - \sqrt{\mathcal{A}_k^2 - \mathcal{B}_k^2})$ joins the constant $\frac{1}{2}\rho^2 \ell^3 \widehat{g}(0) + \frac{1}{2}\rho^2 \ell^3 \widehat{g\omega}(0)$ from $\mathcal{K}$ to give the right energy to LHY precision.

## Treating $\mathcal{Q}_3 = \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L} \widehat{w}_1(k)(a_s^\dagger a_{s-k} a_k + a_k^\dagger a_{s-k}^\dagger a_s)$

$$a_{s-k} a_k = \frac{1}{1-\alpha_k^2}\frac{1}{1-\alpha_{s-k}^2}\Big( b_{s-k} b_k - \alpha_k b_{-k}^\dagger b_{s-k} - \alpha_{s-k} b_{k-s}^\dagger b_k + \alpha_k \alpha_{s-k} b_{k-s}^\dagger b_{-k}^\dagger - \alpha_k [b_{s-k}, b_{-k}^\dagger] \Big).$$

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So,

$$\sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \mathcal{Q}_3 \approx \sum_{k\in P_H}\mathcal{D}_k b_k^\dagger b_k + \ell^{-3}\sqrt{n}\sum_{k\in P_H, s\in P_L}\widehat{w}_1(k)(a_s^\dagger b_{s-k}b_k + b_k^\dagger b_{s-k}^\dagger a_s)$$

$$= \sum_{k\in P_H}\mathcal{D}_k\Big(b_k^\dagger + \ell^{-3}\sqrt{n}\frac{\widehat{w}_1(k)}{\mathcal{D}_k}\sum_{s\in P_L}a_s^\dagger b_{s-k}\Big)\Big(b_k + \ell^{-3}\sqrt{n}\frac{\widehat{w}_1(k)}{\mathcal{D}_k}\sum_{s'\in P_L}b_{s'-k}^\dagger a_{s'}\Big)$$

$$-2\frac{n}{\ell^6}\sum_{k\in P_H}\frac{\widehat{w}_1(k)^2}{2\mathcal{D}_k}\sum_{s\in P_L}a_s^\dagger b_{s-k}\sum_{s'\in P_L}b_{s'-k}^\dagger a_{s'}.$$

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$$- 2\frac{n}{\ell^6}\sum_{k\in P_H}\frac{\widehat{w}_1(k)^2}{2\mathcal{D}_k}\sum_{s\in P_L} a_s^\dagger b_{s-k} \sum_{s'\in P_L} b_{s'-k}^\dagger a_{s'}.$$

Notice that $\ell^{-3}\sum_{k\in P_H}\frac{\widehat{w}_1(k)^2}{2\mathcal{D}_k} \approx \widehat{g\omega}(0)$ and $[b_{s-k}, b_{s'-k}^\dagger] \approx \delta_{s,s'}$. Therefore, this term takes out $\mathcal{Q}_2^{\rm ex}$.